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6. AUTHOR(S)
Dana D. Dlott

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Fredrick Seitz Materials Research Laboratory
University of Illinois at Urbana Champaign

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13. ABSTRACT (Maximum 200 words)

The proposer requested funding for laser equipment that would be used to study engineered nanometric energetic materials consisting of nanometer metal particles, passivation layers and oxidizing binders. The laser equipment is set up for vibrational sum-frequency generation spectroscopy, which looks at the vibrational transitions of molecules at interfaces between metal particles, their passivation layer and the surrounding oxidizer, in real time while the material is being combusted by a carbon dioxide laser. Interface spectroscopy is crucial because almost all of the relevant chemistry in nanoenergetic materials occurs at interfaces. The needed equipment was ordered and installed, and assembled into a working SFG set up that has been tested on a model system consisting of a self assembled monolayer of alkane on gold. The next step will be to finish integrating the carbon dioxide laser system and to begin looking at aluminum based energetic materials.

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1. LIST OF MANUSCRIPTS

none

2. SCIENTIFIC PERSONNEL

James Patterson, graduate assistant
Alex Lagoutchev, postdoctoral associate
Zhaohui Wang, postdoctoral associate

3. REPORT OF INVENTIONS

none

4. SCIENTIFIC PROGRESS AND ACCOMPLISHMENTS

Chemistry of nanoenergetic materials is to a large extent fast interfacial thermochemistry. The idea of this research is to measure the detailed molecular processes occurring at the interfaces between metal particles, metal oxide passivation layers and oxidizers. The technique that will be used is termed "vibrational sum-frequency generation" spectroscopy (SFG). This technique is a surface or interface selective probe of molecular vibrational transitions.

The original research plan called for us to synthesize engineered nanometric energetic materials based on shape selected aluminum nanoparticles with organic monolayer passivation embedded in three dimensional arrays of oxidizing binders. These new materials would be combusted using a high power carbon dioxide laser, while the dynamical processes occurring at the interfaces were monitored in real time using SFG. However the DURINT program was able to provide only equipment support. For this reason, the revised research plan calls for us to first set up and test this fast combustion—surface apparatus. We then intend to look at simplified but relevant model systems that can easily be prepared with a minimum of effort, such as aluminum thin films (planar geometry) with various passivation layers including oxides and self-assembled monolayers. The carbon dioxide laser will be used to burn off the passivation layer while its chemistry is monitored using SFG. It is hoped that support can eventually be found for a full scale synthetic and theoretical effort to synthesize novel nanoenergetic materials and understand their chemical dynamics.

Purchasing this laser equipment took a lot of effort and time. Since the funding was awarded on May 1, 2001, we requested bids, placed the order, had the equipment manufactured and had it installed. Final installation occurred in mid Dec, 2001. At the time this report is written, the installed equipment has been available for only a few weeks. Nevertheless, we have determined that the new mid infrared laser is readily tunable throughout the 2.5 to 20 micron range and it produces more than adequate power. This is important because we wish to key into molecular vibrations of the type Al-F and Al-O which occur around 8-14 microns which was not accessible until now. We obtained a test SFG spectrum on a well known sample consisting of a long chain alkane on a gold surface. We have gotten the carbon dioxide combustion system working reasonably well. We hope to be studying fast energetic material combustion in the next few months with this new system.

This new equipment is fabulous and its acquisition represents a major step forward for this research program. Our deepest gratitude is expressed to the ARO DURINT program for the opportunity to participate.

Equipment acquired

1. High power picosecond laser amplifier
2. Visible and near-IR optical parametric amplifier for narrow band SFG experiments
3. Broadband femtosecond mid-IR optical parametric amplifier for broad band SFG experiments

4. Gated intensified charge-coupled array detector and spectrograph for detecting SFG signals
5. Optical mounts and optical components needed to steer the laser beams